Lattice Boltzmann models based on Gauss quadratures

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Boltzmann Equation

- Evolution equation of the one-particle distribution function $f \equiv f(\mathbf{x}, \mathbf{p})$

$$\partial_t f + \frac{1}{m} p_\alpha \partial_\alpha f = J[f], \qquad J \text{ describes inter-particle collisions}$$

- Hydrodynamic moments give macroscopic quantities:

number density: $$n = \int d^3p\, f,$$

velocity: $$\mathbf{u} = \frac{1}{nm} \int d^3p\, f\, \mathbf{p},$$

temperature: $$T = \frac{1}{3nm} \int d^3p\, f\, \boldsymbol{\xi}^2, \qquad (\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u}),$$

heat flux: $$\mathbf{q} = \frac{1}{2m^2} \int d^3p\, f\, \boldsymbol{\xi}^2\, \boldsymbol{\xi}.$$

Collision terms

- Single relaxation collision term:

$$J[f] = -\frac{1}{\tau}[f - g], \qquad \tau = \frac{\mathrm{Kn}}{n} \text{ is the relaxation time.}$$

- f is relaxing towards g
- Shakhov collision model:

$$g = f^{(\mathrm{eq})}\left\{1 + \frac{1-\mathrm{Pr}}{nT^2}\left[\frac{\boldsymbol{\xi}^2}{(D+2)mT} - 1\right]\boldsymbol{\xi}\cdot\mathbf{q}\right\}, \qquad \mathbf{q} \text{ is the heat flux.}$$

- $\mathrm{Pr} = 2/3$ for an ideal gas
- The BGK model $g = f^{(\mathrm{eq})}$ is recovered when $\mathrm{Pr} = 1$.
- $f^{(\mathrm{eq})}$ is the Maxwell-Boltzmann distribution function:

$$f^{(\mathrm{eq})} = \frac{n}{(2\pi mT)^{D/2}}\exp\left(-\frac{\boldsymbol{\xi}^2}{2mT}\right) \qquad (\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u})$$

Macroscopic quantities and moments of $f^{(\mathrm{eq})}$

- Chapman-Enskog expansion gives f in terms of $f^{(\mathrm{eq})}$:

$$\begin{aligned} f =& f^{(\mathrm{eq})} + \mathrm{Kn}\, f^{(1)} + \mathrm{Kn}^2 f^{(2)} + \dots, \\ \partial_t =& \partial_{t_0} + \mathrm{Kn}\, \partial_{t_1} + \mathrm{Kn}^2 \partial_{t_2} + \dots, \\ \tau =& \mathrm{Kn} \times \frac{\tau}{\mathrm{Kn}}. \end{aligned}$$

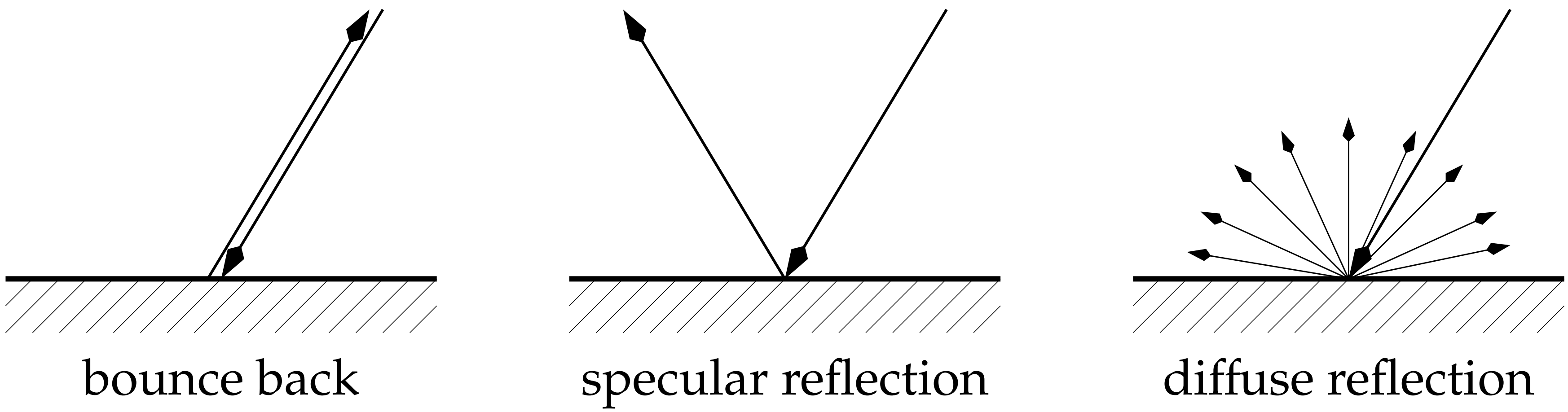
- From $\partial_t f + \frac{\mathbf{p}}{m} \nabla f = -\frac{1}{\tau}(f - g)$:

$$f^{(0)} = g^{(0)}, \qquad f^{(1)} = g^{(1)} - \frac{\tau}{\mathrm{Kn}} \left(\partial_{t_0} + \frac{\mathbf{p}}{m} \nabla \right) f^{(0)}, \qquad \text{etc.}$$

- The recovery of the energy equation at Navier-Stokes-Fourier level requires moments of $f^{(\mathrm{eq})}$ of order 4 for BGK ($g^{(0)} = f^{(\mathrm{eq})}, g^{(1)} = 0$) and of order 6 for Shakhov.

Boundary conditions for the distribution function

Due to the particle – wall interaction, reflected particles carry some information that belongs to the wall.



diffuse reflection the distribution function of *reflected* particles is identical to the Maxwellian distribution function $f^{(eq)}(\mathbf{u}_{\text{wall}}, T_{\text{wall}})$

microfluidics $\text{Kn} = \lambda / L$ is non-negligible

$\Rightarrow$ velocity slip u_{slip}

$\Rightarrow$ temperature jump T_{jump}

Diffuse reflection boundary conditions

The evolution eq. gives the outgoing/incoming fluxes $\mathcal{F}^{out}_{kji\alpha}(\mathbf{x}, t)$ and $\mathcal{F}^{in}_{kji\alpha}(\mathbf{x}, t)$:

$$f_{kji}(\mathbf{x}, t + \delta t) = f_{kji}(\mathbf{x}, t) - \sum_{\alpha} \frac{p_{kji\alpha}}{m} \frac{\delta t}{\delta s} \left[\mathcal{F}^{out}_{kji\alpha}(\mathbf{x}, t) - \mathcal{F}^{in}_{kji\alpha}(\mathbf{x}, t)\right] - \frac{\delta t}{\tau} \left\{f_{kji}(\mathbf{x}, t) - f^{(\mathrm{eq})}_{kji}(\mathbf{x}, t)\left[1 + S_{kji}(\mathbf{x}, t)\right]\right\}$$

The incoming flux on the boundary is given by:

$$\mathcal{F}^{in}_{kji\alpha}(\mathbf{x}_b, t) = -f^{(eq)}(n_w, u_w, T_w) p_{kji\alpha} = -n_w F_k(T_w) E_{kji}(\mathbf{u}_w, T_w) p_{kji\alpha},$$

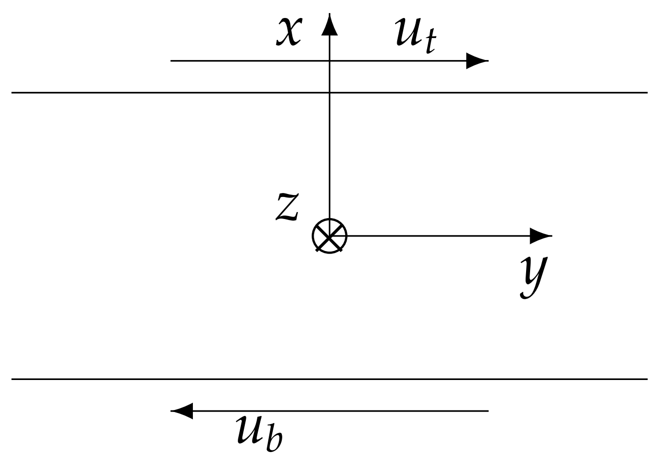
with n_w computed using half-space integrals

$$n_w = \frac{\displaystyle\int_{\mathbf{p}\cdot\boldsymbol{\chi}>0} f(\mathbf{x}_w, t)\,\mathbf{p}\cdot\boldsymbol{\chi}\, d^D p}{(\beta_w/\pi)^{D/2} \displaystyle\int_{\mathbf{p}\cdot\boldsymbol{\chi}<0} e^{-\beta_w(\mathbf{p}-m\mathbf{u}_w)^2}\,\mathbf{p}\cdot\boldsymbol{\chi}\, d^D p} = -\frac{\displaystyle\sum_{p_{kji\alpha}>0} \mathcal{F}^{out}_{kji\alpha}(\mathbf{x}_b, t)}{\displaystyle\sum_{p_{kji\alpha}<0} F_k(T_w) E_{kji}(\mathbf{u}_w, T_w) p_{kji\alpha}}$$

Ansumali and Karlin, Physical Review E **66** (2002) 026311; Meng and Zhang, Physical Review E **83** (2011) 036704

Application: Couette flow

- flow between parallel plates moving along the y axis
- $x_t = -x_b = 0.5$
- Velocity of plates: $u_t = -u_b = 0.42$
- Temperature of plates: $T_b = T_t = 1.0$
- Number of nodes: $n_x = 100$, $n_y = n_z = 2$
- Lattice spacing: $\delta s = 1/100$
- Time step: $\delta t = 10^{-4}$
- Periodic boundary conditions on the y and z axes
- Diffuse reflection boundary conditions on the x axis
- *MCD* flux limiter scheme for $p_\alpha \partial_\alpha$



Simulations done using PETSc 3.1 at:

- NANOSIM cluster - collaboration with Prof. Daniel Vizman, West University of Timişoara, Romania
- IBM-SP6, CINECA - collaboration with Prof. Giuseppe Gonnella, University of Bari, Italy
- MATRIX system, CASPUR - collaboration with dr. Antonio Lamura, IAC-CNR, Section of Bari, Italy
- BlueGene cluster - collaboration with Prof. Daniela Petcu, West University of Timişoara, Romania

Cartesian and spherical coordinates: HLB and SLB

- The accuracy of LB models is given by the moments of $f^{(\mathrm{eq})}$ that they recover.
- The Hermite $HLB(N; Q_x, Q_y, Q_z)$ models use the Cartesian coordinates:

$$\int_{-\infty}^{\infty} dp_\alpha f^{(\mathrm{eq})}(p_\alpha) p_\alpha^{n_\alpha} \to \sum_{k=1}^{Q_\alpha} f^{(\mathrm{eq})}(p_{\alpha,k}) p_{\alpha,k}^{n_\alpha}.$$

- The spherical $SLB(N; K, L, M)$ models use quadratures along:

$$\text{The azimuth: } \int_0^{2\pi} d\varphi\, f^{(\mathrm{eq})} P_n(p, \theta, \varphi) = \sum_{i=1}^{M} \frac{2\pi}{M} f_i^{(\mathrm{eq})} P_n(p, \theta, \varphi_i),$$

$$\text{The elevation: } \int_{-1}^{1} d\cos\theta\, f_i^{(\mathrm{eq})} P_n(p, \theta, \varphi_i) = \sum_{j=1}^{Q} w_j^P f_{ji}^{(\mathrm{eq})} P_n(p, \theta_j, \varphi_i),$$

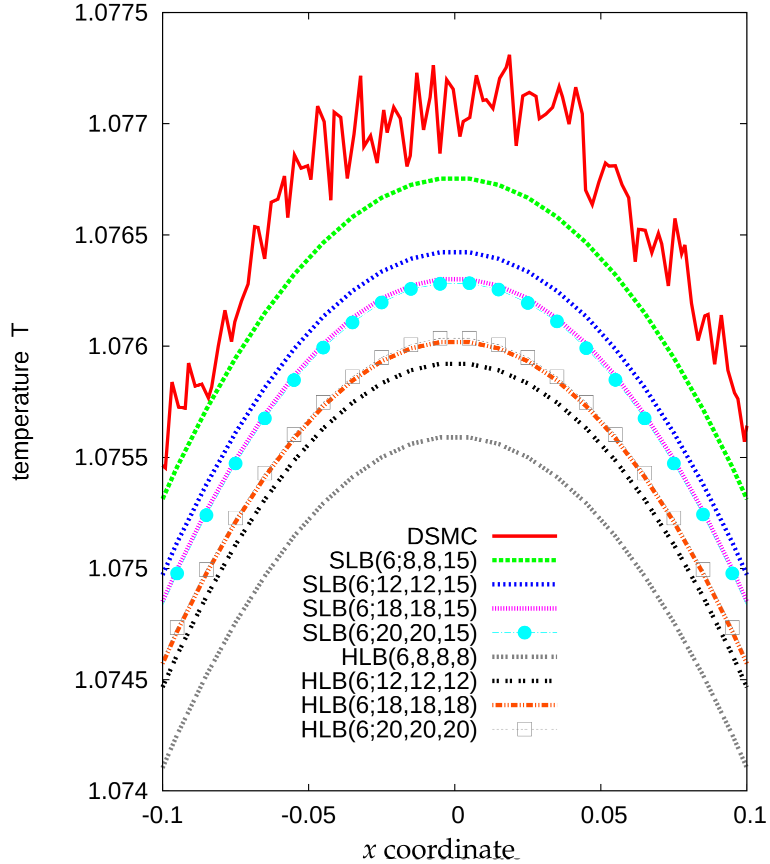
$$\text{The magnitude } p\text{: } \int_0^{\infty} p^2\, dp\, f_{ji}^{(\mathrm{eq})} P_n(p, \theta_j, \varphi_i) = \sum_{k=1}^{K} w_k^L e^{p_k^2} f_{kji}^{(\mathrm{eq})} P_n(p_k, \theta_j, \varphi_i).$$

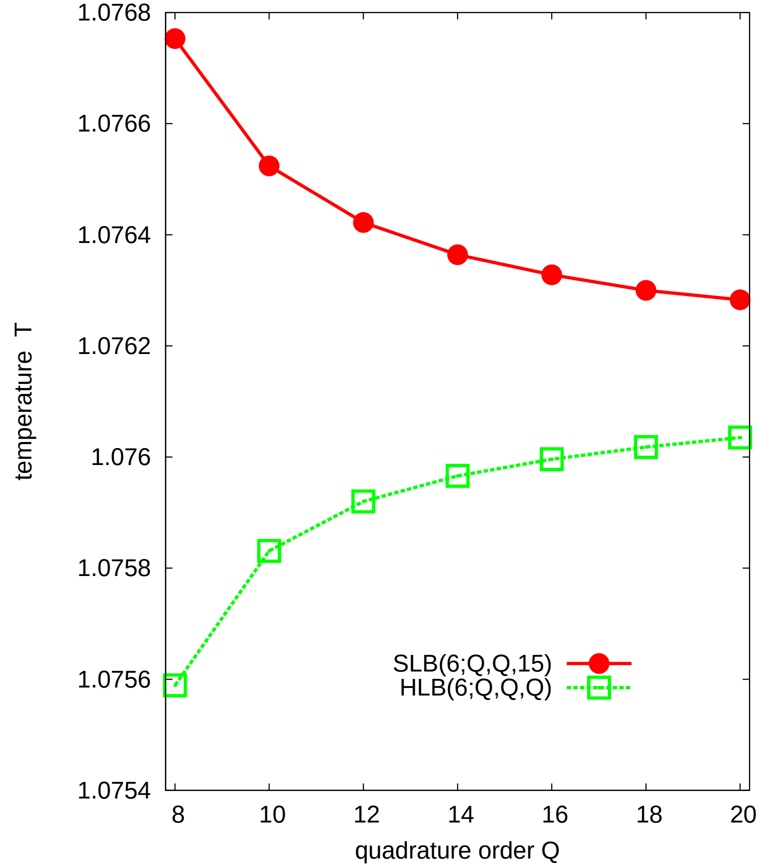
X.Shan, X.-F.Yuan and H.Chen, J. Fluid Mech. (2006), **550**, 413–441

V.E.Ambruş and V.Sofonea, Phys.Rev.E (2012), **86**, 016708

Performance of HLB and SLB models

Convergence of the temperature value in the center of the channel





- *HLB* and *SLB* do not recover exactly half-space integrals.
- High order quadratures are needed to get accurate results for Kn $\gtrsim 0.1$.
- Large velocity sets increase computational costs $\Rightarrow$ poor numerical stability.

Exact recovery of half-space integrals

- Strategy: use an integration method which explicitly deals with half-moments
- Solution: split the $3D$ momentum space into octants:

$$\int d^3p\, g(\mathbf{p}) = \int_0^\infty dp_x \int_0^\infty dp_y \int_0^\infty dp_z\, [g(+,+,+) + g(+,+,-) + \dots],$$
$$g(+,-,-) \equiv g(p_x, -p_y, -p_z), \text{ etc.}$$

- The integration domain $[0, \infty)$ is amenable to the Gauss-Laguerre quadrature method ($2Q_\alpha > n$):

$$\int_0^\infty dp_\alpha\, e^{-p_\alpha} P_n(p_\alpha) = \sum_{k=1}^{Q_\alpha} w_{\alpha,k} P_n(p_{\alpha,k})$$

- Now integrals over octants are exactly recovered, giving an accurate implementation of diffuse reflection boundary conditions

V. E. Ambruş and V. Sofonea, paper in preparation

Construction of LLB: expansion of $f^{(\mathrm{eq})}$

- The distribution function is split into $f^{\pm} = f(\pm|p_\alpha|)$:

$$\int_{-\infty}^{\infty} dp_\alpha f(p_\alpha) P_n(p_\alpha) = \sum_{k=1}^{Q_\alpha} w_{\alpha,k} e^{p_{\alpha,k}} \left[f^+(p_{\alpha,k}) P_n(p_{\alpha,k}) + f^-(p_{\alpha,k}) P_n(-p_{\alpha,k}) \right]$$

- The equilibrium distribution function in LLB models is factorized as:

$$f^{(\mathrm{eq})} = n g_x g_y g_z, \qquad g_\alpha(p_\alpha; u_\alpha, T) = \sqrt{\frac{1}{2\pi m T}} \exp\left[-\frac{(p_\alpha - m u_\alpha)^2}{2mT} \right]$$

- g_α can be expanded with respect to the Laguerre polynomials:

$$g_\alpha = e^{-|p_\alpha|} \sum_{\ell=0}^{Q_\alpha - 1} \mathcal{G}_{\alpha,\ell}(u_\alpha, T) L_\ell(|p_\alpha|),$$

$$\mathcal{G}_{\alpha,\ell} = \frac{1}{2} \sum_{s=0}^{\ell} \frac{(-1)^s}{s!} \binom{\ell}{s} \left(\frac{mT}{2} \right)^{\frac{s}{2}} \left[(1 + \mathrm{erf}\zeta_\alpha) P_s(\zeta_\alpha) + \frac{2}{\sqrt{\pi}} e^{-\zeta_\alpha^2} P_s^*(\zeta_\alpha) \right],$$

where $P_s(\zeta_\alpha)$ and $P_s^*(\zeta_\alpha)$ are polynomials of order s in $\zeta_\alpha = u_\alpha \sqrt{\frac{m}{2T}}$.

E. P. Gross, E. A. Jackson and S. Ziering, Annals of Physics, **1**, 141-167 (1957)

Discretisation of the momentum space

- The Gauss-Laguerre quadrature gives:

$$\int_{-\infty}^{\infty} dp_\alpha f(p_\alpha) P_n(p_\alpha) \to \sum_{k=1}^{Q_\alpha} e^{p_{\alpha.k}} w_{\alpha,k} [f(p_{\alpha,k}) P_n(p_{\alpha,k}) + f(-p_{\alpha,k}) P_n(-p_{\alpha,k})]$$

Discretisation of the momentum space

- The Gauss-Laguerre quadrature gives:

$$\int_{-\infty}^{\infty} dp_\alpha f(p_\alpha) P_n(p_\alpha) \to \sum_{k=1}^{2Q_\alpha} e^{|p_{\alpha,k}|} w_{\alpha,k} f(p_{\alpha,k}) P_n(p_{\alpha,k})$$

- The velocity set and quadrature weights are given by:

$$p_{\alpha,k} = \begin{cases} k\text{'th root of } L_{Q_\alpha} & k \le Q_\alpha, \\ -p_{\alpha,k-Q_\alpha} & k > Q_\alpha \end{cases}, \qquad w_{\alpha,k} = \frac{|p_{\alpha,k}|}{(Q_\alpha+1)^2 \left[L_{Q_\alpha+1}(|p_{\alpha,k}|)\right]^2}.$$

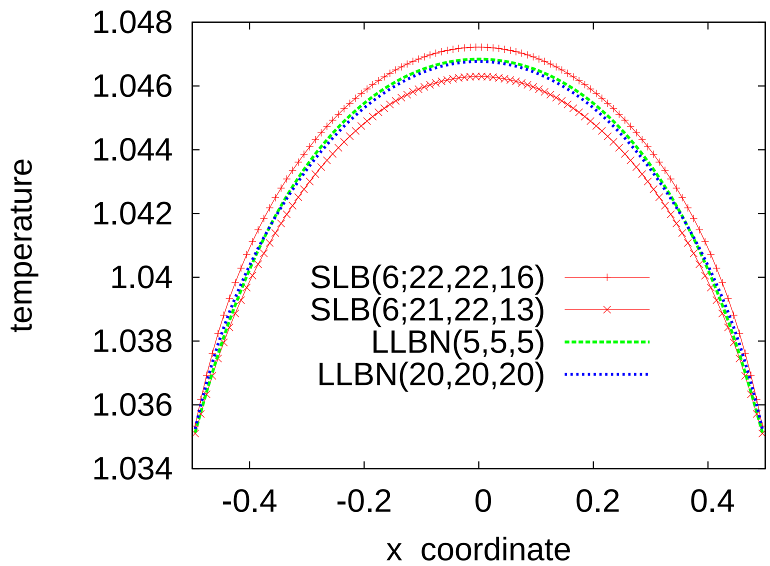
- Defining $g_{\alpha,k} = w_{\alpha,k} e^{-|p_{\alpha,k}|} g_\alpha(p_{\alpha,k})$, the moments of f are replaced by:

$$\int d^3p\, f\, P_n(\mathbf{p}) \to \sum_{i=1}^{2Q_x} \sum_{j=1}^{2Q_y} \sum_{k=1}^{2Q_z} f_{ijk} P_n(\mathbf{p}_{ijk}), \qquad f_{ijk} = n g_{x,i} g_{y,j} g_{z,k}.$$

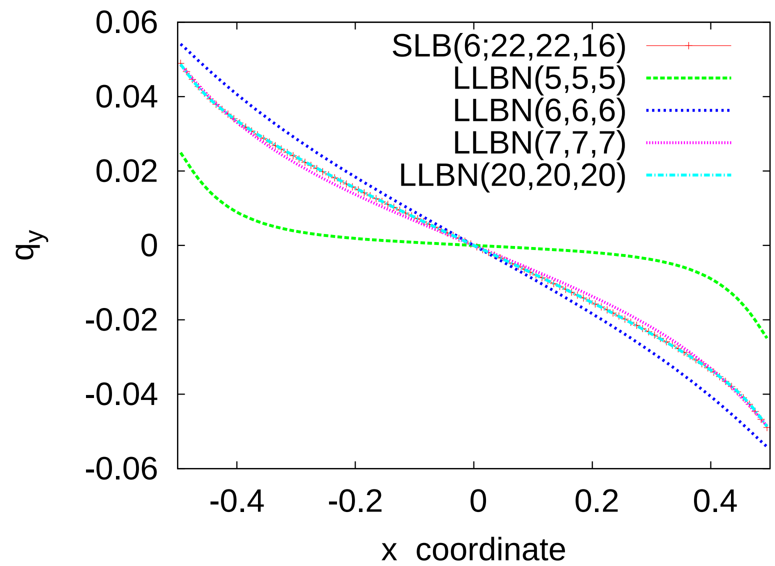
- The Gauss quadrature rules require $Q_\alpha > N \Rightarrow 8(N+1)^3$ momentum vectors required for N'th order accuracy.

LLBN vs SLB: Numeric results for Couette flow at Kn=0.5

Temperature profile



Transversal heat flux

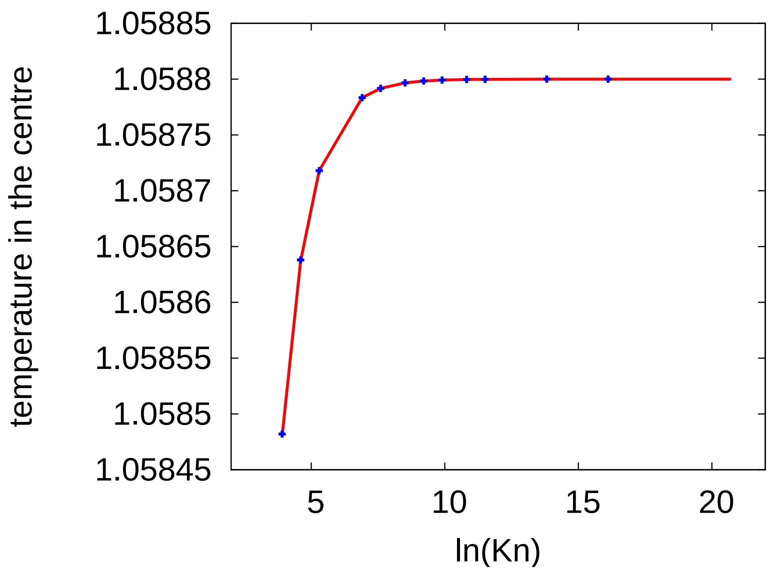


$Q = 7$ ($N = 6$) needed to recover the NSF equations in the Shakhov model.

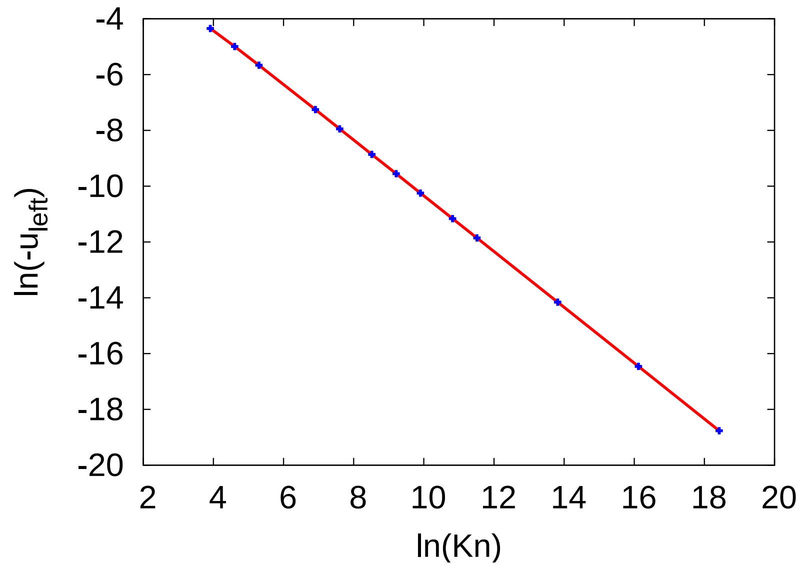
$$(u_{walls} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-5} \ , \ Kn = 0.5)$$

Large Kn explorations using LLBN

Temperature in the centre of the channel



Logarithm of velocity at the wall



- At high Kn, BGK and Shakhov behave similarly
- The balistic regime is accurately captured, even for temperature differences of order $T_{\text{right}} - T_{\text{left}} \sim 10$.

$$(u_{walls} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-5} \ , \ Q_x = 21)$$

Conclusion

- The Laguerre (LLB) models exactly recover half-space moments of $f^{(\mathrm{eq})}$, which are crucial for the implementation of diffuse reflection boundary conditions.
- The LLB models in Couette flow are stable at large Kn (up to 10^9) and accurately capture the Balistic regime.
- The LLB models are stable in systems with large temperature differences (differences up to 10 tested).